

5 **WHAT IS CLAIMED IS:**

1. A research method performed for carrying out a set of experiments, the method comprising:

10 providing to a remote user at a first location a computer-implemented experiment design tool for generating an experiment design defining a set of experiments, the experiment design including an experiment matrix having a plurality of matrix elements, one or more starting materials assigned to the matrix elements and one or more process conditions to be applied to the matrix elements, each of a plurality of matrix elements being defined by a unique combination of starting materials and/or process conditions, the experiment design also defining a screening method to be applied to generate experimental results;

15 receiving at a second location a first user input including a first experiment design generated by the experiment design tool, the second location being remote from the first location;

preparing a library of materials corresponding to the experiment matrix, the library of materials having a plurality of members;

20 applying the process conditions to the members of the library of materials to transform at least one of the starting materials into a product;

applying a first screening method defined by the first experiment design to generate experimental results; and

25 providing the experimental results to the remote user.

2. The method of claim 1, wherein:

30 the first screening method is a high throughput screening method.

3. The method of claim 2, wherein:

35 the first screening method is selected from the group consisting of infrared thermography, chromatography, capillary electrophoresis, mass spectrometry, optical reflection, optical transmission, viscometry, mechanical resonators, solubility, differential scanning calorimetry, elongation, indentation, deformation or spectroscopy.

35 4. The method of claim 2, wherein:

5        the experiment matrix includes at least 50 elements; and  
the experimental results are provided to the user within 20 days from preparation of the  
first library.

10      5.      The method of claim 2, wherein:  
the experiment matrix includes at least 96 elements; and  
the experimental results are provided to the user within 10 days from preparation of the  
first library.

6.      The method of claim 2, wherein:  
the experiment matrix includes at least 1000 elements; and  
the experimental results are provided to the user within 50 days from preparation of the  
first library.

7.      The method of claim 2, wherein:  
the experiment matrix includes at least 1000 elements; and  
the experimental results are provided to the user within 20 days from preparation of the  
first library.

8.      The method of claim 2, wherein:  
the experiment matrix includes at least 1000 elements; and  
the experimental results are provided to the user within 10 days from preparation of the  
first library.

9.      The method of claim 2, further comprising:  
30      in response to providing the experimental results, receiving a second user input including  
a second experiment design defining one or more additional experiments;  
preparing a second library of materials based on the second experiment design;  
applying one or more process conditions specified in the second experiment design to the  
members of the second library of materials to transform at least one of the starting materials into  
35      a product and applying a second screening method to generate additional experimental results;

5 and

providing the additional experimental results to the remote user.

10. The method of claim 9, wherein:

the second library of materials is a superset of the first library of materials.

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11. The method of claim 9, wherein:

the second screening method and the first screening method are different.

12. The method of claim 2, wherein:

the computer-implemented experiment design tool includes an interactive user interface configured to enable the remote user to select materials from a list of materials in a remote material inventory.

13. The method of claim 2, wherein:

the computer-implemented experiment design tool includes an interactive user interface configured to enable the user to select processing conditions from a list of processing conditions that can be implemented by a remote process control system.

14. The method of claim 2, wherein:

the computer-implemented experiment design tool includes an interactive user interface configured to enable the user to select high throughput screening methods from a list of screening methods that can be performed by one or more screening instruments available at a remote laboratory location.

30 15. The method of claim 2, wherein:

the computer-implemented experiment design tool includes an interactive user interface configured to access one or more databases of available materials, process conditions and high throughput screening methods.

35 16. The method of claim 2, wherein:

5 the first screening method is automatically defined based on one or more of the starting materials and process conditions.

17. The method of claim 2, further comprising:  
evaluating the first experiment design before preparing the library of materials to generate  
10 an experimental plan describing a proposed execution of the set of experiments; and  
providing the experimental plan to the remote user.

18. The method of claim 17, wherein:  
evaluating the first experiment design includes generating an estimate of time and/or cost  
to perform the set of experiments defined by the first experiment design.

19. The method of claim 17, wherein:  
evaluating the first experiment design includes determining whether the design conforms to a set of experiment parameters, and, if not, communicating to the remote user that one or more experiments defined by the experiment design cannot be executed.

20. The method of claim 19, wherein:  
determining whether the design conforms to the set of experiment parameters includes  
determining whether the assigned starting materials specified in the first experiment design are  
present in an inventory of materials.

21. The method of claim 19, wherein:  
evaluating the first experiment design includes determining whether the assigned starting  
materials have chemical or physical properties falling within a predetermined set of chemical or  
30 physical properties.

22. The method of claim 1, wherein:  
the computer-implemented experiment design tool is configured to enable the remote user  
to generate an experiment request for execution of the set of experiments defined by the first  
35 experiment design for submission over a computer network.

5

23. The method of claim 22, wherein:

the first experiment design is received from the remote user over a computer network.

10 24. The method of claim 1, wherein:

the first experiment design includes information identifying one or more custom materials assigned to one or more matrix elements; the method further comprising:

receiving the custom materials from the remote user for use in preparing the library of materials.

15 25. The method of claim 1, wherein:

the first experiment design defines a set of experiments directed to chemcatalysis or biocatalysis.

20 26. The method of claim 1, wherein:

the first experiment design defines a set of experiments directed to optimization of a chemical synthetic process.

27. The method of claim 26, wherein:

the set of experiments is directed to the preparation of pharmaceutical products or intermediates.

28. The method of claim 26, wherein:

the set of experiments is directed to the preparation of fine chemicals.

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29. The method of claim 26, wherein:

the set of experiments is directed to the preparation of specialty chemicals.

35 30. The method of claim 26, wherein:

the set of experiments is directed to the preparation of commodity chemicals

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31. The method of claim 1, wherein:

the first experiment design defines a set of experiments directed to polymerization.

32. The method of claim 31, wherein:

10 the set of experiments is directed to the preparation of polymeric coatings, adhesives, dispersants, surfactants or additives.

33. The method of claim 1, wherein:

15 the first experiment design defines a set of experiments directed to the preparation of electronic materials.

34. The method of claim 1, wherein:

20 the experiment design defines a set of experiments directed to the preparation of composites or alloys.

35. The method of claim 2, wherein:

25 the user receives the experimental results by accessing a results database through a remote computer-implemented interactive user interface.

36. The method of claim 2, further comprising:

30 in response to providing the experimental results, receiving a second user input from the remote user including a request to purchase a starting material or product corresponding to one of the elements of the experiment matrix.

37. The method of claim 1, wherein:

35 the experiment design tool is provided as a computer program to be executed by a computer system at the first location.

38. The method of claim 1, wherein:

35 the experiment design tool is provided as a computer program executed by a server

5 process running at the second location; and

the remote user accesses the experiment design tool using a client process running at the first location.

39. A method for obtaining experimental results for a set of experiments, the method

10 comprising:

generating at a first location an experiment design defining a set of experiments, the experiment design including an experiment matrix having a plurality of elements, one or more starting materials assigned to the matrix elements, and one or more process conditions to be applied to the matrix elements, each of a plurality of matrix elements being defined by a unique combination of starting materials and/or process conditions, the experiment design also defining a screening method to be applied to generate experimental results;

communicating the experiment design to a laboratory at a second location for execution, the second location being remote from the first location;

receiving at the first location an experimental plan describing a proposed execution of the set of experiments;

if the proposed execution of the set of experiments is acceptable, communicating an approval of the experimental plan to the laboratory; and

receiving at the first location experimental results obtained at the laboratory by applying the process conditions to a library of materials corresponding to the experiment matrix to transform at least one of the starting materials into a product and applying the specified screening method.

40. The method of claim 39, wherein:

the experimental plan includes an estimate of time and/or cost to perform the set of

30 experiments.

41. A computer-implemented method for designing a set of experiments for execution by a remote laboratory, comprising:

defining an experiment matrix having a plurality of matrix elements corresponding to

35 locations in a library of materials;

5 designating one or more starting materials and assigning each starting material to one or more matrix elements, and designating at least one processing condition to be applied to one or more elements of the experiment matrix, such that each of a plurality of matrix elements is defined by a unique combination of starting materials and/or process conditions;

10 designating a screening method to be applied to one or more elements of the experiment matrix; and

communicating an experiment design to the remote laboratory, the experiment design including the experiment matrix and the screening method designation.

42. The method of claim 41, wherein:

15 the starting materials are selected from a list of materials in a remote material inventory.

43. The method of claim 41, wherein:

the processing conditions are selected from a list of processing conditions that can be implemented by a remote process control system.

44. The method of claim 41, wherein:

the screening method is selected from a list of screening methods that can be performed by one or more remote screening instruments.

45. The method of claim 41, wherein:

the screening method is automatically defined based on one or more of the starting materials and process conditions.

46. The method of claim 41, wherein:

30 the experiment design is communicated to the remote laboratory over a computer network.

47. A computer-implemented research system for carrying out a set of experiments, comprising:

35 a computer-implemented remote experiment design tool for generating an experiment

5 design defining a set of experiments, the experiment design including an experiment matrix having a plurality of matrix elements, one or more starting materials assigned to the matrix elements and one or more process conditions to be applied to the matrix elements, each of a plurality of matrix elements being defined by a unique combination of starting materials and/or process conditions, the experiment design also defining a screening method to be applied to 10 generate experimental results;

a user interface subsystem configured to receive an experiment design generated by the experiment design tool and to provide experimental results to a user; and

15 a research engine configured to evaluate the experiment design, generate an experimental plan describing a proposed execution of the set of experiments, and prepare a library of materials corresponding to the experiment matrix according to the experimental plan, the library of materials having a plurality of members, each member containing the starting materials assigned to a corresponding matrix element, the research engine being operable to apply the process conditions to the members of the library of materials to transform at least one of the starting materials into a product and to apply the screening method to generate experimental results.

48. The system of claim 47, further comprising:

an inventory subsystem including an inventory database storing information identifying a plurality of materials in a material inventory.

49. The system of claim 47, further comprising:

one or more automated instruments coupled to the research engine; and

wherein the research engine includes a process database storing information identifying a plurality of chemical processes capable of being performed by the one or more automated instruments.

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50. The system of claim 47, wherein:

the research engine includes an experiment database storing information about one or more sets of experiments executed on behalf of the remote user.

35 51. A computer-readable storage medium tangibly embodying a research system program, the

5 program comprising instructions operable to cause a programmable processor to:

provide to a remote user at a first location a computer-implemented experiment design tool for generating an experiment design defining a set of experiments, the experiment design including an experiment matrix having a plurality of matrix elements, one or more starting materials assigned to the matrix elements and one or more process conditions to be applied to the 10 matrix elements, each of a plurality of matrix elements being defined by a unique combination of starting materials and/or process conditions, the experiment design also defining a screening method to be applied to generate experimental results;

receive at a second location a first user input including an experiment design generated by the experiment design tool, the second location being remote from the first location;

15 direct an automated synthesis instrument to prepare a library of materials corresponding to the experiment matrix, the library of materials having a plurality of members;

direct an automated instrument to apply the process conditions to the members of the library of materials to transform at least one of the starting materials into a product;

direct an automated screening instrument to apply a first screening method defined by the first experiment design to generate experimental results; and

provide the experimental results to the remote user.

52. A computer-readable storage medium tangibly embodying a program for designing a set of experiments for execution by a remote laboratory, the program comprising instructions operable to cause a programmable processor to:

25 receive an input defining an experiment matrix having a plurality of matrix elements corresponding to locations in a library of materials;

receive an input designating one or more starting materials and assigning each starting material to one or more matrix elements, and designating at least one processing condition to be applied to one or more elements of the experiment matrix, such that each of a plurality of matrix 30 elements is defined by a unique combination of starting materials and/or process conditions;

receive an input designating a screening method to be applied to one or more elements of the experiment matrix; and

communicate an experiment design to the remote laboratory, the experiment design including the experiment matrix and the screening method designation.